

## Author index

- Abematsu, C., see Nakayama, H. 253 (2000) 331
- Abram, U., see Voigt, A. 253 (2000) 171
- Adachi, H., see Suzuki, C. 253 (2000) 27
- Agostini, G., L. Pasimeni, M. Ruzzi, S. Monti, M. Maggini, M. Prato, I. Lamparth and A. Hirsch, Fullerene derivatives embedded in poly(methylmethacrylate): a laser flash photolysis and time-resolved EPR study 253 (2000) 105
- Alemán, C., The keto–amino/enol tautomerism of cytosine in aqueous solution. A theoretical study using combined discrete/self-consistent reaction field models 253 (2000) 13
- Aramendia, P.F., see Torga, J.R. 253 (2000) 249
- Böttcher, R., see Voigt, A. 253 (2000) 171
- Badenes, M.P., E. Castellano, C.J. Cobos, A.E. Croce and M.E. Tucceri, Kinetics of the reactions of  $\text{FC(O)O}_2$  radicals with F atoms and  $\text{F}_2$  253 (2000) 205
- Bakker, H.J., see van den Broek, M.A.F.H. 253 (2000) 157
- Bartolotti, L.J., see Chesnut, D.B. 253 (2000) 1
- Bergman, D.L., Topological properties of the hydrogen-bond network in liquid water 253 (2000) 267
- Bhattacharyya, S.P., see Chaudhury, P. 253 (2000) 295
- Bielschowsky, C.E., see Rocha, A.B. 253 (2000) 51
- Boulet, P., F. Gilardoni, J. Weber, H. Chermette and Y. Ellinger, Reply to Comment on “Theoretical study of interstellar hydroxylamine chemistry: protonation and proton transfer mediated by  $\text{H}_3^+$ ” [Chem. Phys. 253 (2000) 389–390] 253 (2000) 391
- Brion, C.E., see Litvinyuk, I.V. 253 (2000) 41
- Buehler, E.J., E.E. Gooch, J.L. Dial and S.K. Knudson, Semiclassical energies of low-lying states of one-electron diatomics 253 (2000) 219
- Cacace, F., and G. de Petris, Comment on “Theoretical study of interstellar hydroxylamine chemistry: protonation and proton transfer mediated by  $\text{H}_3^+$ ” [Chem. Phys. 244 (2000) 163–174] 253 (2000) 389
- Castellano, E., see Badenes, M.P. 253 (2000) 205
- Chaudhury, P., S.P. Bhattacharyya and W. Quapp, A genetic algorithm based technique for locating first-order saddle point using a gradient dominated recipe 253 (2000) 295
- Chermette, H., see Boulet, P. 253 (2000) 391
- Chesnut, D.B., and L.J. Bartolotti, The electron localization function description of aromaticity in five-membered rings 253 (2000) 1
- Cobos, C.J., see Badenes, M.P. 253 (2000) 205

- Croce, A.E., see Badenes, M.P. 253 (2000) 205
- da Silveira, N.P., F.S. Rodembusch, F.V. Pereira, D. Samios and P.R. Livotto, Ab initio determination of the  $C_6H_6 \cdots CS_2$  cluster stabilization energy 253 (2000) 165
- de Petris, G., see Cacace, F. 253 (2000) 389
- Dial, J.L., see Buehler, E.J. 253 (2000) 219
- Doktorov, A.B., see Toropov, Yu.V. 253 (2000) 231
- Edvardsson, D., see Holland, D.M.P. 253 (2000) 133
- Ellinger, Y., see Boulet, P. 253 (2000) 391
- Fourkas, J.T., see Loughnane, B.J. 253 (2000) 323
- Franco, M.L., see Jorge, F.E. 253 (2000) 21
- Fritzsche, S., R. Haberlandt and M. Wolfsberg, Equilibration of the kinetic energy in small zeolite cavities. The thermalization effect of lattice vibrations and of mutual interaction in the diffusion of methane in a cation-free LTA zeolite 253 (2000) 283
- Fujimoto, H., see Kimura, T. 253 (2000) 125
- Gómez, J.A., and D. Guenzburger, Density functional study of electronic, magnetic and hyperfine properties of  $[M(CN)_5NO]^{2-}$  ( $M = Fe, Ru$ ) and reduction products 253 (2000) 73
- Gilardoni, F., see Boulet, P. 253 (2000) 391
- Gooch, E.E., see Buehler, E.J. 253 (2000) 219
- Guenzburger, D., see Gómez, J.A. 253 (2000) 73
- Guo, S.-L., see Zhu, X.-L. 253 (2000) 241
- Haberlandt, R., see Fritzsche, S. 253 (2000) 283
- Halkier, A., B. Kirchner, H. Huber and M. Jaszuński, Nuclear quadrupole coupling constant of  $^{21}Ne$  in the neon dimer and its influence on the  $T_1$  NMR relaxation time in fluid neon 253 (2000) 183
- Hashimoto, Y., see Kimura, T. 253 (2000) 125
- Hirsch, A., see Agostini, G. 253 (2000) 105
- Holland, D.M.P., D. Edvardsson, L. Karlsson, R. Maripuu, K. Siegbahn, A.W. Potts and W. von Niessen, A systematic investigation of the influence of Cooper minima on the photoionisation dynamics of the monohalobenzenes 253 (2000) 133
- Huber, H., see Halkier, A. 253 (2000) 183
- Hupp, J.T., see Vance, F.W. 253 (2000) 313
- Ishii, K., see Nakayama, H. 253 (2000) 331
- Izvekov, V., see Kovács, A. 253 (2000) 193
- Jaszuński, M., see Halkier, A. 253 (2000) 183
- Jorge, F.E., and M.L. Franco, A universal Gaussian basis set for positive and negative ions from H through Xe 253 (2000) 21
- Jurczok, M., P. Plaza, M.M. Martin, Y.H. Meyer and W. Rettig, Excited state relaxation paths in 9,9'-bianthryl and 9-carbazolyl-anthracene: a sub-ps transient absorption study 253 (2000) 339
- Karlsson, L., see Holland, D.M.P. 253 (2000) 133
- Kawai, J., see Suzuki, C. 253 (2000) 27

- Keresztury, G., see Kovács, A. 253 (2000) 193
- Kim, H.-S., Monte Carlo simulation study of solvent effect on Na<sup>+</sup> to Li<sup>+</sup> ion mutation 253 (2000) 305
- Kimura, T., M. Sumimoto, S. Sakaki, H. Fujimoto, Y. Hashimoto and S. Matsuzaki, Electronic structure of lithium phthalocyanine studied by ultraviolet photoemission spectroscopy 253 (2000) 125
- Kirchner, B., see Halkier, A. 253 (2000) 183
- Kirmse, R., see Voigt, A. 253 (2000) 171
- Knudson, S.K., see Buehler, E.J. 253 (2000) 219
- Kosuge, M., see Moriyama, M. 253 (2000) 91
- Kovács, A., G. Keresztury and V. Izvekov, Intramolecular hydrogen-bonding in 2-nitroresorcinol. A combined FT-IR, FT-Raman and computational study 253 (2000) 193
- Kovačević, B., see Maksić, Z.B. 253 (2000) 59
- Lamparth, I., see Agostini, G. 253 (2000) 105
- Lesar, A., see Maksić, Z.B. 253 (2000) 59
- Litvinyuk, I.V., Y. Zheng and C.E. Brion, Valence shell orbital imaging in adamantane by electron momentum spectroscopy 253 (2000) 41
- Livotto, P.R., see da Silveira, N.P. 253 (2000) 165
- Loughnane, B.J., A. Scodinu and J.T. Fourkas, Temperature-dependent optical Kerr effect spectroscopy of chloroform in restricted geometries 253 (2000) 323
- Maggini, M., see Agostini, G. 253 (2000) 105
- Makarov, V.I., and E. Quiñones, Relaxation of individual rotational levels of the  $\tilde{A}^1A_u$  electronic state of acetylene excited to the  $2\nu_3$  and  $(\nu'_1+\nu'_3+\nu'_6)$  vibrational modes 253 (2000) 259
- Maksić, Z.B., B. Kovačević and A. Lesar, Protonation of archetypal aromatic and antiaromatic systems – G2 studies of benzene and cyclobutadiene 253 (2000) 59
- Mandal, A.K., and M.K. Pal, Strong fluorescence emissions by H-aggregates of the dye thiacyanine in the presence of the surfactant aerosol-OT 253 (2000) 115
- Marconi, M.C., see Torga, J.R. 253 (2000) 249
- Maripuu, R., see Holland, D.M.P. 253 (2000) 133
- Martin Negri, R., see Torga, J.R. 253 (2000) 249
- Martin, M.M., see Jurczok, M. 253 (2000) 339
- Matsuzaki, S., see Kimura, T. 253 (2000) 125
- Meyer, Y.H., see Jurczok, M. 253 (2000) 339
- Mihailović, D., see Umek, P. 253 (2000) 361
- Minagawa, Y., see Nakayama, H. 253 (2000) 331
- Molin, Yu.N., see Toropov, Yu.V. 253 (2000) 231
- Molinari, E., and M. Tomellini, Non-equilibrium vibrational kinetics in adlayers: outline of an alternative approach to catalytic processes 253 (2000) 367
- Monti, S., see Agostini, G. 253 (2000) 105
- Moriyama, M., M. Kosuge, S. Tobita and H. Shizuka, Excited-state intramolecular proton transfer followed by *cis-trans* isomerization of (1-hydroxy-2-naphthyl)-s-triazine derivatives 253 (2000) 91
- Mukoyama, T., see Suzuki, C. 253 (2000) 27
- Nakayama, H., Y. Minagawa, C. Abematsu, S. Yajima and K. Ishii, Pseudo-lattice vibrations in smectic phase of liquid crystals: studies on small wave number Raman spectra of 4-alkyl-4'-cyanobiphenyl 253 (2000) 331

- Omerzu, A., see Umek, P. 253 (2000) 361
- Painelli, A., Erratum to: "Amplification of NLO responses: vibronic and solvent effects in push-pull polyenes" [Chem. Phys. 245 (2000) 185–197] 253 (2000) 393
- Pal, M.K., see Mandal, A.K. 253 (2000) 115
- Pasimeni, L., see Agostini, G. 253 (2000) 105
- Pereira, F.V., see da Silveira, N.P. 253 (2000) 165
- Plaza, P., see Jurczok, M. 253 (2000) 339
- Potts, A.W., see Holland, D.M.P. 253 (2000) 133
- Prato, M., see Agostini, G. 253 (2000) 105
- Quapp, W., see Chaudhury, P. 253 (2000) 295
- Quiñones, E., see Makarov, V.I. 253 (2000) 259
- Reinhold, J., see Voigt, A. 253 (2000) 171
- Rettig, W., see Jurczok, M. 253 (2000) 339
- Richter, U., see Voigt, A. 253 (2000) 171
- Rocha, A.B., and C.E. Bielschowsky, Vibronic coupling for H<sub>2</sub>CO and CO<sub>2</sub> 253 (2000) 51
- Rodembusch, F.S., see da Silveira, N.P. 253 (2000) 165
- Ruzzi, M., see Agostini, G. 253 (2000) 105
- Saito, N., see Suzuki, I.H. 253 (2000) 351
- Sakaki, S., see Kimura, T. 253 (2000) 125
- Samios, D., see da Silveira, N.P. 253 (2000) 165
- Scodinu, A., see Loughnane, B.J. 253 (2000) 323
- Shizuka, H., see Moriyama, M. 253 (2000) 91
- Siegbahn, K., see Holland, D.M.P. 253 (2000) 133
- Slone, R.V., see Vance, F.W. 253 (2000) 313
- Stass, D.V., see Toropov, Yu.V. 253 (2000) 231
- Stern, C.L., see Vance, F.W. 253 (2000) 313
- Sumimoto, M., see Kimura, T. 253 (2000) 125
- Suzuki, C., J. Kawai, M. Takahashi, A.-M. Vlaicu, H. Adachi and T. Mukoyama, The electronic structure of rare-earth oxides in the creation of the core hole 253 (2000) 27
- Suzuki, I.H., and N. Saito, Energy dependences of fragment ion yields from acetone photoexcited in the C1s and O1s transition regions 253 (2000) 351
- Sviridenko, F.B., see Toropov, Yu.V. 253 (2000) 231
- Takahashi, M., see Suzuki, C. 253 (2000) 27
- Tobita, S., see Moriyama, M. 253 (2000) 91
- Tokumoto, M., see Umek, P. 253 (2000) 361
- Tomellini, M., see Molinari, E. 253 (2000) 367
- Torga, J.R., M.C. Marconi, R. Martín Negri and P.F. Aramendia, Molecular rotational diffusion detected by differential fluorescence energy 253 (2000) 249
- Toropov, Yu.V., F.B. Sviridenko, D.V. Stass, A.B. Doktorov and Yu.N. Molin, Influence of geminate recombination kinetics on the shape of low field MARY line 253 (2000) 231
- Tucceri, M.E., see Badenes, M.P. 253 (2000) 205

- Umek, P., A. Omerzu, D. Mihailović and M. Tokumoto, Synthesis and magnetic characterisation of fullerene derivative based ferromagnets 1-(3-nitro)- and 1-(3-aminophenyl)-1H-methanofullerene doped with cobaltocene 253 (2000) 361
- van den Broek, M.A.F.H., and H.J. Bakker, Observation of a bottleneck in the vibrational relaxation of liquid bromoform 253 (2000) 157
- Vance, F.W., R.V. Slone, C.L. Stern and J.T. Hupp, Comparative absorption, electroabsorption and electrochemical studies of intervalence electron transfer and electronic coupling in cyanide-bridged bimetallic systems: ancillary ligand effects 253 (2000) 313
- Vlaicu, A.-M., see Suzuki, C. 253 (2000) 27
- Voigt, A., U. Abram, R. Böttcher, U. Richter, J. Reinhold and R. Kirmse, Q-Band single-crystal EPR study and molecular orbital calculations of  $[(C_6H_5)_4As][Re^{V}_{VINCl_4}]$  253 (2000) 171
- von Niessen, W., see Holland, D.M.P. 253 (2000) 133
- Weber, J., see Boulet, P. 253 (2000) 391
- Wolfsberg, M., see Fritzsche, S. 253 (2000) 283
- Yajima, S., see Nakayama, H. 253 (2000) 331
- You, X.-Z., see Zhu, X.-L. 253 (2000) 241
- Yu, Z., see Zhu, X.-L. 253 (2000) 241
- Zheng, Y., see Litvinyuk, I.V. 253 (2000) 41
- Zhong, Y., see Zhu, X.-L. 253 (2000) 241
- Zhu, X.-L., X.-Z. You, Y. Zhong, Z. Yu and S.-L. Guo, An improved calculation method on optical second-order susceptibilities of organic materials 253 (2000) 241



## Subject index

### Methods and constructs

#### Theoretical

##### *Computational methods for electronic structure*

- The electron localization function description of aromaticity in five-membered rings,  
D.B. Chesnut and L.J. Bartolotti 253 (2000) 1
- The keto–amino/enol tautomerism of cytosine in aqueous solution. A theoretical study  
using combined discrete/self-consistent reaction field models, C. Alemán 253 (2000) 13
- A universal Gaussian basis set for positive and negative ions from H through Xe,  
F.E. Jorge and M.L. Franco 253 (2000) 21
- The electronic structure of rare-earth oxides in the creation of the core hole, C. Suzuki,  
J. Kawai, M. Takahashi, A.-M. Vlaicu, H. Adachi and T. Mukoyama 253 (2000) 27
- Valence shell orbital imaging in adamantane by electron momentum spectroscopy,  
I.V. Litvinyuk, Y. Zheng and C.E. Brion 253 (2000) 41
- Vibronic coupling for H<sub>2</sub>CO and CO<sub>2</sub>, A.B. Rocha and C.E. Bielschowsky 253 (2000) 51
- Ab initio determination of the C<sub>6</sub>H<sub>6</sub>⋯CS<sub>2</sub> cluster stabilization energy, N.P. da Silveira,  
F.S. Rodembusch, F.V. Pereira, D. Samios and P.R. Livotto 253 (2000) 165
- Q-Band single-crystal EPR study and molecular orbital calculations of [(C<sub>6</sub>H<sub>5</sub>)<sub>4</sub>As]  
[Re<sup>V</sup>1NCl<sub>4</sub>/Re<sup>V</sup>OCl<sub>4</sub>], A. Voigt, U. Abram, R. Böttcher, U. Richter, J. Reinhold and  
R. Kirmse 253 (2000) 171

##### *-CI and valence bond approach*

- Vibronic coupling for H<sub>2</sub>CO and CO<sub>2</sub>, A.B. Rocha and C.E. Bielschowsky 253 (2000) 51

##### *-perturbative and many body approaches*

- Protonation of archetypal aromatic and antiaromatic systems – G2 studies of benzene  
and cyclobutadiene, Z.B. Maksić, B. Kovačević and A. Lesar 253 (2000) 59
- Nuclear quadrupole coupling constant of <sup>21</sup>Ne in the neon dimer and its influence on  
the T<sub>1</sub> NMR relaxation time in fluid neon, A. Halkier, B. Kirchner, H. Huber and  
M. Jaszuński 253 (2000) 183

##### *-density functional theory*

- Density functional study of electronic, magnetic and hyperfine properties of  
[M(CN)<sub>5</sub>NO]<sup>2-</sup> (M = Fe, Ru) and reduction products, J.A. Gómez and  
D. Guenzburger 253 (2000) 73

- Intramolecular hydrogen-bonding in 2-nitroresorcinol. A combined FT-IR, FT-Raman and computational study, A. Kovács, G. Keresztury and V. Izvekov 253 (2000) 193
- Kinetics of the reactions of  $\text{FC(O)O}_2$  radicals with F atoms and  $\text{F}_2$ , M.P. Badenes, E. Castellano, C.J. Cobos, A.E. Croce and M.E. Tucceri 253 (2000) 205
- Semiempirical methods*
- Excited-state intramolecular proton transfer followed by *cis-trans* isomerization of (1-hydroxy-2-naphthyl)-s-triazine derivatives, M. Moriyama, M. Kosuge, S. Tobita and H. Shizuka 253 (2000) 91
- Algebraic approaches*
- Semiclassical energies of low-lying states of one-electron diatomics, E.J. Buehler, E.E. Gooch, J.L. Dial and S.K. Knudson 253 (2000) 219
- Spin states and magnetic interactions*
- Density functional study of electronic, magnetic and hyperfine properties of  $[\text{M}(\text{CN})_5\text{NO}]^{2-}$  ( $\text{M} = \text{Fe}, \text{Ru}$ ) and reduction products, J.A. Gómez and D. Guenzburger 253 (2000) 73
- Fullerene derivatives embedded in poly(methylmethacrylate): a laser flash photolysis and time-resolved EPR study, G. Agostini, L. Pasimeni, M. Ruzzi, S. Monti, M. Maggini, M. Prato, I. Lamparth and A. Hirsch 253 (2000) 105
- Influence of geminate recombination kinetics on the shape of low field MARY line, Yu.V. Toropov, F.B. Sviridenko, D.V. Stass, A.B. Doktorov and Yu.N. Molin 253 (2000) 231
- Molecular response to external fields (incl. optical susceptibilities, dichroism, hyperpolarizabilities)*
- An improved calculation method on optical second-order susceptibilities of organic materials, X.-L. Zhu, X.-Z. You, Y. Zhong, Z. Yu and S.-L. Guo 253 (2000) 241
- Molecular rotational diffusion detected by differential fluorescence energy, J.R. Torga, M.C. Marconi, R. Martín Negri and P.F. Aramendía 253 (2000) 249
- Collisional and reactive molecular dynamics with non-frictional forces*
- Relaxation of individual rotational levels of the  $\tilde{\text{A}}^1\text{A}_u$  electronic state of acetylene excited to the  $2\nu'_3$  and  $(\nu'_1 + \nu'_3 + \nu'_6)$  vibrational modes, V.I. Makarov and E. Quiñones 253 (2000) 259
- Molecular dynamics of many particle systems and condensed phases*
- Nuclear quadrupole coupling constant of  $^{21}\text{Ne}$  in the neon dimer and its influence on the  $T_1$  NMR relaxation time in fluid neon, A. Halkier, B. Kirchner, H. Huber and M. Jaszuński 253 (2000) 183
- Topological properties of the hydrogen-bond network in liquid water, D.L. Bergman 253 (2000) 267
- Migration and interaction on grids and lattices*
- Equilibration of the kinetic energy in small zeolite cavities. The thermalization effect of lattice vibrations and of mutual interaction in the diffusion of methane in a cation-free LTA zeolite, S. Fritzsche, R. Haberlandt and M. Wolfsberg 253 (2000) 283



*Statistical computational methods (incl. Monte Carlo)*

- Kinetics of the reactions of  $\text{FC(O)O}_2$  radicals with F atoms and  $\text{F}_2$ , M.P. Badenes, E. Castellano, C.J. Cobos, A.E. Croce and M.E. Tucceri 253 (2000) 205
- Equilibration of the kinetic energy in small zeolite cavities. The thermalization effect of lattice vibrations and of mutual interaction in the diffusion of methane in a cation-free LTA zeolite, S. Fritzsche, R. Haberlandt and M. Wolfsberg 253 (2000) 283
- A genetic algorithm based technique for locating first-order saddle point using a gradient dominated recipe, P. Chaudhury, S.P. Bhattacharyya and W. Quapp 253 (2000) 295
- Monte Carlo simulation study of solvent effect on  $\text{Na}^+$  to  $\text{Li}^+$  ion mutation, H.-S. Kim 253 (2000) 305

*Extremum methods for ensembles (energy, entropy, free energy)*

- Monte Carlo simulation study of solvent effect on  $\text{Na}^+$  to  $\text{Li}^+$  ion mutation, H.-S. Kim 253 (2000) 305

**Experiment***Magnetic resonances*

- Fullerene derivatives embedded in poly(methylmethacrylate): a laser flash photolysis and time-resolved EPR study, G. Agostini, L. Pasimeni, M. Ruzzi, S. Monti, M. Maggini, M. Prato, I. Lamparth and A. Hirsch 253 (2000) 105
- Q-Band single-crystal EPR study and molecular orbital calculations of  $[(\text{C}_6\text{H}_5)_4\text{As}][\text{Re}^{\text{VI}}\text{NCl}_4/\text{Re}^{\text{V}}\text{OCl}_4]$ , A. Voigt, U. Abram, R. Böttcher, U. Richter, J. Reinhold and R. Kirmse 253 (2000) 171

*Molecular spectroscopy*

- Strong fluorescence emissions by H-aggregates of the dye thiacyanine in the presence of the surfactant aerosol-OT, A.K. Mandal and M.K. Pal 253 (2000) 115
- Comparative absorption, electroabsorption and electrochemical studies of intervalence electron transfer and electronic coupling in cyanide-bridged bimetallic systems: ancillary ligand effects, F.W. Vance, R.V. Slone, C.L. Stern and J.T. Hupp 253 (2000) 313

*-infrared*

- Intramolecular hydrogen-bonding in 2-nitroresorcinol. A combined FT-IR, FT-Raman and computational study, A. Kovács, G. Keresztury and V. Izvekov 253 (2000) 193

*-Raman*

- Intramolecular hydrogen-bonding in 2-nitroresorcinol. A combined FT-IR, FT-Raman and computational study, A. Kovács, G. Keresztury and V. Izvekov 253 (2000) 193
- Temperature-dependent optical Kerr effect spectroscopy of chloroform in restricted geometries, B.J. Loughnane, A. Scodinu and J.T. Fourkas 253 (2000) 323
- Pseudo-lattice vibrations in smectic phase of liquid crystals: studies on small wave number Raman spectra of 4-alkyl-4'-cyanobiphenyl, H. Nakayama, Y. Minagawa, C. Abematsu, S. Yajima and K. Ishii 253 (2000) 331

*-UV*

- An improved calculation method on optical second-order susceptibilities of organic materials, X.-L. Zhu, X.-Z. You, Y. Zhong, Z. Yu and S.-L. Guo 253 (2000) 241

- Relaxation of individual rotational levels of the  $\tilde{A}^1A_u$  electronic state of acetylene excited to the  $2\nu_3$  and  $(\nu_1 + \nu_3 + \nu_6)$  vibrational modes, V.I. Makarov and E. Quir6nes 253 (2000) 259
- Photon counting and phase fluorimetry*
- Excited-state intramolecular proton transfer followed by *cis-trans* isomerization of (1-hydroxy-2-naphthyl)-s-triazine derivatives, M. Moriyama, M. Kosuge, S. Tobita and H. Shizuka 253 (2000) 91
- Strong fluorescence emissions by H-aggregates of the dye thiacyanine in the presence of the surfactant aerosol-OT, A.K. Mandal and M.K. Pal 253 (2000) 115
- Photoelectron and Auger spectroscopy*
- Electronic structure of lithium phthalocyanine studied by ultraviolet photoemission spectroscopy, T. Kimura, M. Sumimoto, S. Sakaki, H. Fujimoto, Y. Hashimoto and S. Matsuzaki 253 (2000) 125
- A systematic investigation of the influence of Cooper minima on the photoionisation dynamics of the monohalobenzenes, D.M.P. Holland, D. Edvardsson, L. Karlsson, R. Maripuu, K. Siegbahn, A.W. Potts and W. von Niessen 253 (2000) 133
- X-ray spectroscopy*
- The electronic structure of rare-earth oxides in the creation of the core hole, C. Suzuki, J. Kawai, M. Takahashi, A.-M. Vlaicu, H. Adachi and T. Mukoyama 253 (2000) 27
- Electron impact spectroscopy*
- Valence shell orbital imaging in adamantane by electron momentum spectroscopy, I.V. Litvinyuk, Y. Zheng and C.E. Brion 253 (2000) 41
- Ultrafast measurements*
- Observation of a bottleneck in the vibrational relaxation of liquid bromoform, M.A.F.H. van den Broek and H.J. Bakker 253 (2000) 157
- Molecular rotational diffusion detected by differential fluorescence energy, J.R. Torga, M.C. Marconi, R. Mart6n Negri and P.F. Aramendia 253 (2000) 249
- Excited state relaxation paths in 9,9'-bianthryl and 9-carbazolyl-anthracene: a sub-ps transient absorption study, M. Jurczok, P. Plaza, M.M. Martin, Y.H. Meyer and W. Rettig 253 (2000) 339
- Synchrotron spectroscopies*
- A systematic investigation of the influence of Cooper minima on the photoionisation dynamics of the monohalobenzenes, D.M.P. Holland, D. Edvardsson, L. Karlsson, R. Maripuu, K. Siegbahn, A.W. Potts and W. von Niessen 253 (2000) 133
- Energy dependences of fragment ion yields from acetone photoexcited in the C1s and O1s transition regions, I.H. Suzuki and N. Saito 253 (2000) 351
- Atomic and molecular beam techniques*
- Relaxation of individual rotational levels of the  $\tilde{A}^1A_u$  electronic state of acetylene excited to the  $2\nu_3$  and  $(\nu_1 + \nu_3 + \nu_6)$  vibrational modes, V.I. Makarov and E. Quir6nes 253 (2000) 259

*Mass spectroscopy*

- Protonation of archetypal aromatic and antiaromatic systems – G2 studies of benzene and cyclobutadiene, Z.B. Maksić, B. Kovačević and A. Lesar 253 (2000) 59
- Energy dependences of fragment ion yields from acetone photoexcited in the C1s and O1s transition regions, I.H. Suzuki and N. Saito 253 (2000) 351

*Radiolysis*

- Influence of geminate recombination kinetics on the shape of low field MARY line, Yu.V. Toropov, F.B. Sviridenko, D.V. Stass, A.B. Doktorov and Yu.N. Molin 253 (2000) 231

*Measurement of macroscopic variables*

- Kinetics of the reactions of  $\text{FC}(\text{O})\text{O}_2$  radicals with F atoms and  $\text{F}_2$ , M.P. Badenes, E. Castellano, C.J. Cobos, A.E. Croce and M.E. Tucceri 253 (2000) 205
- Synthesis and magnetic characterisation of fullerene derivative based ferromagnets 1-(3-nitro)- and 1-(3-aminophenyl)-1H-methanofullerene doped with cobaltocene, P. Umek, A. Omerzu, D. Mihailović and M. Tokumoto 253 (2000) 361

**Objects****Bulk systems***Gases*

- The electron localization function description of aromaticity in five-membered rings, D.B. Chesnut and L.J. Bartolotti 253 (2000) 1
- Protonation of archetypal aromatic and antiaromatic systems – G2 studies of benzene and cyclobutadiene, Z.B. Maksić, B. Kovačević and A. Lesar 253 (2000) 59
- Kinetics of the reactions of  $\text{FC}(\text{O})\text{O}_2$  radicals with F atoms and  $\text{F}_2$ , M.P. Badenes, E. Castellano, C.J. Cobos, A.E. Croce and M.E. Tucceri 253 (2000) 205
- Relaxation of individual rotational levels of the  $\tilde{\text{A}}^1\text{A}_u$  electronic state of acetylene excited to the  $2\nu'_3$  and  $(\nu'_1 + \nu'_3 + \nu'_6)$  vibrational modes, V.I. Makarov and E. Quiñones 253 (2000) 259

*Liquids neat*

- Observation of a bottleneck in the vibrational relaxation of liquid bromoform, M.A.F.H. van den Broek and H.J. Bakker 253 (2000) 157
- Topological properties of the hydrogen-bond network in liquid water, D.L. Bergman 253 (2000) 267
- Temperature-dependent optical Kerr effect spectroscopy of chloroform in restricted geometries, B.J. Loughnane, A. Scodinu and J.T. Fourkas 253 (2000) 323

*Liquid mixtures and solutions*

- Excited-state intramolecular proton transfer followed by *cis-trans* isomerization of (1-hydroxy-2-naphthyl)-s-triazine derivatives, M. Moriyama, M. Kosuge, S. Tobita and H. Shizuka 253 (2000) 91
- Molecular rotational diffusion detected by differential fluorescence energy, J.R. Torga, M.C. Marconi, R. Martin Negri and P.F. Aramendia 253 (2000) 249
- Excited state relaxation paths in 9,9'-bianthryl and 9-carbazolyl-anthracene: a sub-ps transient absorption study, M. Jurczok, P. Plaza, M.M. Martin, Y.H. Meyer and W. Rettig 253 (2000) 339

*Crystals*

- An improved calculation method on optical second-order susceptibilities of organic materials, X.-L. Zhu, X.-Z. You, Y. Zhong, Z. Yu and S.-L. Guo 253 (2000) 241
- Equilibration of the kinetic energy in small zeolite cavities. The thermalization effect of lattice vibrations and of mutual interaction in the diffusion of methane in a cation-free LTA zeolite, S. Fritzsche, R. Haberlandt and M. Wolfsberg 253 (2000) 283

*-neat*

- An improved calculation method on optical second-order susceptibilities of organic materials, X.-L. Zhu, X.-Z. You, Y. Zhong, Z. Yu and S.-L. Guo 253 (2000) 241

*-mixed*

- Synthesis and magnetic characterisation of fullerene derivative based ferromagnets 1-(3-nitro)- and 1-(3-aminophenyl)-1*H*-methanofullerene doped with cobaltocene, P. Umek, A. Omerzu, D. Mihailović and M. Tokumoto 253 (2000) 361

*Complex fluids*

- Topological properties of the hydrogen-bond network in liquid water, D.L. Bergman 253 (2000) 267

*-liquid crystals*

- Pseudo-lattice vibrations in smectic phase of liquid crystals: studies on small wave number Raman spectra of 4-alkyl-4'-cyanobiphenyl, H. Nakayama, Y. Minagawa, C. Abematsu, S. Yajima and K. Ishii 253 (2000) 331

*-micelles*

- Strong fluorescence emissions by H-aggregates of the dye thiacyanine in the presence of the surfactant aerosol-OT, A.K. Mandal and M.K. Pal 253 (2000) 115

*Polymers*

- Fullerene derivatives embedded in poly(methylmethacrylate): a laser flash photolysis and time-resolved EPR study, G. Agostini, L. Pasimeni, M. Ruzzi, S. Monti, M. Maggini, M. Prato, I. Lamparth and A. Hirsch 253 (2000) 105

*Semiconductors*

- Electronic structure of lithium phthalocyanine studied by ultraviolet photoemission spectroscopy, T. Kimura, M. Sumimoto, S. Sakaki, H. Fujimoto, Y. Hashimoto and S. Matsuzaki 253 (2000) 125

*Surfaces*

- Temperature-dependent optical Kerr effect spectroscopy of chloroform in restricted geometries, B.J. Loughnane, A. Scodinu and J.T. Fourkas 253 (2000) 323

*Biological systems*

- The keto-amino/enol tautomerism of cytosine in aqueous solution. A theoretical study using combined discrete/self-consistent reaction field models, C. Alemán 253 (2000) 13

**Microscopic and mesoscopic systems***Molecules (neutral and ionic)*

- The electron localization function description of aromaticity in five-membered rings,  
D.B. Chesnut and L.J. Bartolotti 253 (2000) 1
- The electronic structure of rare-earth oxides in the creation of the core hole, C. Suzuki,  
J. Kawai, M. Takahashi, A.-M. Vlaicu, H. Adachi and T. Mukoyama 253 (2000) 27
- Molecular rotational diffusion detected by differential fluorescence energy, J.R. Torga,  
M.C. Marconi, R. Martin Negri and P.F. Aramendia 253 (2000) 249
- Comparative absorption, electroabsorption and electrochemical studies of intervalence  
electron transfer and electronic coupling in cyanide-bridged bimetallic systems:  
ancillary ligand effects, F.W. Vance, R.V. Slone, C.L. Stern and J.T. Hupp 253 (2000) 313

*-diatomic*

- Nuclear quadrupole coupling constant of  $^{21}\text{Ne}$  in the neon dimer and its influence on  
the  $T_1$  NMR relaxation time in fluid neon, A. Halkier, B. Kirchner, H. Huber and  
M. Jaszuński 253 (2000) 183
- Semiclassical energies of low-lying states of one-electron diatomics, E.J. Buehler,  
E.E. Gooch, J.L. Dial and S.K. Knudson 253 (2000) 219

*-small polyatomics*

- The electron localization function description of aromaticity in five-membered rings,  
D.B. Chesnut and L.J. Bartolotti 253 (2000) 1
- Observation of a bottleneck in the vibrational relaxation of liquid bromoform,  
M.A.F.H. van den Broek and H.J. Bakker 253 (2000) 157
- Temperature-dependent optical Kerr effect spectroscopy of chloroform in restricted  
geometries, B.J. Loughnane, A. Scodinu and J.T. Fourkas 253 (2000) 323
- Energy dependences of fragment ion yields from acetone photoexcited in the C1s and  
O1s transition regions, I.H. Suzuki and N. Saito 253 (2000) 351

*-aromatics*

- The electron localization function description of aromaticity in five-membered rings,  
D.B. Chesnut and L.J. Bartolotti 253 (2000) 1
- Protonation of archetypal aromatic and antiaromatic systems – G2 studies of benzene  
and cyclobutadiene, Z.B. Maksić, B. Kovačević and A. Lesar 253 (2000) 59
- A systematic investigation of the influence of Cooper minima on the photoionisation  
dynamics of the monohalobenzenes, D.M.P. Holland, D. Edvardsson, L. Karlsson,  
R. Maripuu, K. Siegbahn, A.W. Potts and W. von Niessen 253 (2000) 133

*-other large*

- Valence shell orbital imaging in adamantane by electron momentum spectroscopy,  
I.V. Litvinyuk, Y. Zheng and C.E. Brion 253 (2000) 41

*Molecular aggregates*

- Fullerene derivatives embedded in poly(methylmethacrylate): a laser flash photolysis  
and time-resolved EPR study, G. Agostini, L. Pasimeni, M. Ruzzi, S. Monti,  
M. Maggini, M. Prato, I. Lamparth and A. Hirsch 253 (2000) 105

- Strong fluorescence emissions by H-aggregates of the dye thiocyanine in the presence of the surfactant aerosol-OT, A.K. Mandal and M.K. Pal 253 (2000) 115
- van der Waals molecules*
- Ab initio determination of the  $C_6H_6 \cdots CS_2$  cluster stabilization energy, N.P. da Silveira, F.S. Rodembusch, F.V. Pereira, D. Samios and P.R. Livotto 253 (2000) 165
- clusters*
- Ab initio determination of the  $C_6H_6 \cdots CS_2$  cluster stabilization energy, N.P. da Silveira, F.S. Rodembusch, F.V. Pereira, D. Samios and P.R. Livotto 253 (2000) 165
- A genetic algorithm based technique for locating first-order saddle point using a gradient dominated recipe, P. Chaudhury, S.P. Bhattacharyya and W. Quapp 253 (2000) 295
- complexes*
- Density functional study of electronic, magnetic and hyperfine properties of  $[M(CN)_5NO]^{2-}$  ( $M = Fe, Ru$ ) and reduction products, J.A. Gómez and D. Guenzburger 253 (2000) 73
- Q-Band single-crystal EPR study and molecular orbital calculations of  $[(C_6H_5)_4As][Re^{VI}NCl_4/Re^{VO}Cl_4]$ , A. Voigt, U. Abram, R. Böttcher, U. Richter, J. Reinhold and R. Kirmse 253 (2000) 171
- Free radicals (incl. hydronium and muonium)*
- Electronic structure of lithium phthalocyanine studied by ultraviolet photoemission spectroscopy, T. Kimura, M. Sumimoto, S. Sakaki, H. Fujimoto, Y. Hashimoto and S. Matsuzaki 253 (2000) 125
- Kinetics of the reactions of  $FC(O)O_2$  radicals with F atoms and  $F_2$ , M.P. Badenes, E. Castellano, C.J. Cobos, A.E. Croce and M.E. Tucceri 253 (2000) 205
- Influence of geminate recombination kinetics on the shape of low field MARY line, Yu.V. Toropov, F.B. Sviridenko, D.V. Stass, A.B. Doktorov and Yu.N. Molin 253 (2000) 231
- Ions and charge carriers*
- A universal Gaussian basis set for positive and negative ions from H through Xe, F.E. Jorge and M.L. Franco 253 (2000) 21
- Influence of geminate recombination kinetics on the shape of low field MARY line, Yu.V. Toropov, F.B. Sviridenko, D.V. Stass, A.B. Doktorov and Yu.N. Molin 253 (2000) 231
- Nucleic acids*
- The keto–amino/enol tautomerism of cytosine in aqueous solution. A theoretical study using combined discrete/self-consistent reaction field models, C. Alemán 253 (2000) 13

## Phenomena

### Molecular structure

- The keto–amino/enol tautomerism of cytosine in aqueous solution. A theoretical study using combined discrete/self-consistent reaction field models, C. Alemán 253 (2000) 13



*Vibrations and rotations of molecules*

- Pseudo-lattice vibrations in smectic phase of liquid crystals: studies on small wave number Raman spectra of 4-alkyl-4'-cyanobiphenyl, H. Nakayama, Y. Minagawa, C. Abematsu, S. Yajima and K. Ishii 253 (2000) 331

*Electronic structure and states*

- A universal Gaussian basis set for positive and negative ions from H through Xe, F.E. Jorge and M.L. Franco 253 (2000) 21
- The electronic structure of rare-earth oxides in the creation of the core hole, C. Suzuki, J. Kawai, M. Takahashi, A.-M. Vlaicu, H. Adachi and T. Mukoyama 253 (2000) 27
- Valence shell orbital imaging in adamantane by electron momentum spectroscopy, I.V. Litvinyuk, Y. Zheng and C.E. Brion 253 (2000) 41
- Vibronic coupling for H<sub>2</sub>CO and CO<sub>2</sub>, A.B. Rocha and C.E. Bielschowsky 253 (2000) 51
- Density functional study of electronic, magnetic and hyperfine properties of [M(CN)<sub>5</sub>NO]<sup>2-</sup> (M = Fe, Ru) and reduction products, J.A. Gómez and D. Guenzburger 253 (2000) 73
- Electronic structure of lithium phthalocyanine studied by ultraviolet photoemission spectroscopy, T. Kimura, M. Sumimoto, S. Sakaki, H. Fujimoto, Y. Hashimoto and S. Matsuzaki 253 (2000) 125
- A systematic investigation of the influence of Cooper minima on the photoionisation dynamics of the monohalobenzenes, D.M.P. Holland, D. Edvardsson, L. Karlsson, R. Maripuu, K. Siegbahn, A.W. Potts and W. von Niessen 253 (2000) 133
- Semiclassical energies of low-lying states of one-electron diatomics, E.J. Buehler, E.E. Gooch, J.L. Dial and S.K. Knudson 253 (2000) 219
- Synthesis and magnetic characterisation of fullerene derivative based ferromagnets 1-(3-nitro)- and 1-(3-aminophenyl)-1H-methanofullerene doped with cobaltocene, P. Umek, A. Omerzu, D. Mihailović and M. Tokumoto 253 (2000) 361

*Electric and magnetic properties*

- Density functional study of electronic, magnetic and hyperfine properties of [M(CN)<sub>5</sub>NO]<sup>2-</sup> (M = Fe, Ru) and reduction products, J.A. Gómez and D. Guenzburger 253 (2000) 73
- Q-Band single-crystal EPR study and molecular orbital calculations of [(C<sub>6</sub>H<sub>5</sub>)<sub>4</sub>As][Re<sup>VI</sup>NCl<sub>4</sub>/Re<sup>V</sup>OCl<sub>4</sub>], A. Voigt, U. Abram, R. Böttcher, U. Richter, J. Reinhold and R. Kirmse 253 (2000) 171
- Nuclear quadrupole coupling constant of <sup>21</sup>Ne in the neon dimer and its influence on the T<sub>1</sub> NMR relaxation time in fluid neon, A. Halkier, B. Kirchner, H. Huber and M. Jaszuński 253 (2000) 183

*Molecular interactions*

- Ab initio determination of the C<sub>6</sub>H<sub>6</sub> ··· CS<sub>2</sub> cluster stabilization energy, N.P. da Silveira, F.S. Rodembusch, F.V. Pereira, D. Samios and P.R. Livotto 253 (2000) 165
- Equilibration of the kinetic energy in small zeolite cavities. The thermalization effect of lattice vibrations and of mutual interaction in the diffusion of methane in a cation-free LTA zeolite, S. Fritzsche, R. Haberlandt and M. Wolfsberg 253 (2000) 283
- Monte Carlo simulation study of solvent effect on Na<sup>+</sup> to Li<sup>+</sup> ion mutation, H.-S. Kim 253 (2000) 305

*Spectral bandshapes and intensities*

- Vibronic coupling for H<sub>2</sub>CO and CO<sub>2</sub>, A.B. Rocha and C.E. Bielschowsky 253 (2000) 51

*Coupling of electronic and nuclear motion*

- Influence of geminate recombination kinetics on the shape of low field MARY line, Yu.V. Toropov, F.B. Sviridenko, D.V. Stass, A.B. Doktorov and Yu.N. Molin 253 (2000) 231

*Molecular photophysical processes*

- Fullerene derivatives embedded in poly(methylmethacrylate): a laser flash photolysis and time-resolved EPR study, G. Agostini, L. Pasimeni, M. Ruzzi, S. Monti, M. Maggini, M. Prato, I. Lamparth and A. Hirsch 253 (2000) 105
- Strong fluorescence emissions by H-aggregates of the dye thiacyanine in the presence of the surfactant aerosol-OT, A.K. Mandal and M.K. Pal 253 (2000) 115
- A systematic investigation of the influence of Cooper minima on the photoionisation dynamics of the monohalobenzenes, D.M.P. Holland, D. Edvardsson, L. Karlsson, R. Maripuu, K. Siegbahn, A.W. Potts and W. von Niessen 253 (2000) 133
- Excited state relaxation paths in 9,9'-bianthryl and 9-carbazolyl-anthracene: a sub-ps transient absorption study, M. Jurczok, P. Plaza, M.M. Martin, Y.H. Meyer and W. Rettig 253 (2000) 339
- Energy dependences of fragment ion yields from acetone photoexcited in the C1s and O1s transition regions, I.H. Suzuki and N. Saito 253 (2000) 351

*Intramolecular dynamics**-radiationless transitions*

- Excited-state intramolecular proton transfer followed by *cis-trans* isomerization of (1-hydroxy-2-naphthyl)-s-triazine derivatives, M. Moriyama, M. Kosuge, S. Tobita and H. Shizuka 253 (2000) 91
- Relaxation of individual rotational levels of the  $\tilde{A}^1A_u$  electronic state of acetylene excited to the  $2\nu_3$  and  $(\nu_1 + \nu_3 + \nu_6)$  vibrational modes, V.I. Makarov and E. Quiñones 253 (2000) 259

*-vibrational energy redistribution (incl. vibrational dissociation)*

- Observation of a bottleneck in the vibrational relaxation of liquid bromoform, M.A.F.H. van den Broek and H.J. Bakker 253 (2000) 157

*Nonlinear responses (incl. optical)*

- An improved calculation method on optical second-order susceptibilities of organic materials, X.-L. Zhu, X.-Z. You, Y. Zhong, Z. Yu and S.-L. Guo 253 (2000) 241

*Reactions (incl. dissociation)*

- A genetic algorithm based technique for locating first-order saddle point using a gradient dominated recipe, P. Chaudhury, S.P. Bhattacharyya and W. Quapp 253 (2000) 295

*Electron transfer*

- Comparative absorption, electroabsorption and electrochemical studies of intervalence electron transfer and electronic coupling in cyanide-bridged bimetallic systems: ancillary ligand effects, F.W. Vance, R.V. Slone, C.L. Stern and J.T. Hupp 253 (2000) 313



- Excited state relaxation paths in 9,9'-bianthryl and 9-carbazolyl-anthracene: a sub-ps transient absorption study, M. Jurczok, P. Plaza, M.M. Martin, Y.H. Meyer and W. Rettig 253 (2000) 339
- Proton and hydrogen atom transfer*
- Protonation of archetypal aromatic and antiaromatic systems – G2 studies of benzene and cyclobutadiene, Z.B. Maksić, B. Kovačević and A. Lesar 253 (2000) 59
- Excited-state intramolecular proton transfer followed by *cis-trans* isomerization of (1-hydroxy-2-naphthyl)-s-triazine derivatives, M. Moriyama, M. Kosuge, S. Tobita and H. Shizuka 253 (2000) 91
- Ionization (incl. Rydberg states)*
- Energy dependences of fragment ion yields from acetone photoexcited in the C1s and O1s transition regions, I.H. Suzuki and N. Saito 253 (2000) 351
- Molecular motion (incl. diffusive)*
- Molecular rotational diffusion detected by differential fluorescence energy, J.R. Torga, M.C. Marconi, R. Martín Negri and P.F. Aramendia 253 (2000) 249
- Pseudo-lattice vibrations in smectic phase of liquid crystals: studies on small wave number Raman spectra of 4-alkyl-4'-cyanobiphenyl, H. Nakayama, Y. Minagawa, C. Abematsu, S. Yajima and K. Ishii 253 (2000) 331
- Collective motion and excitations*
- Pseudo-lattice vibrations in smectic phase of liquid crystals: studies on small wave number Raman spectra of 4-alkyl-4'-cyanobiphenyl, H. Nakayama, Y. Minagawa, C. Abematsu, S. Yajima and K. Ishii 253 (2000) 331
- Surface chemical physics*
- Non-equilibrium vibrational kinetics in adlayers: outline of an alternative approach to catalytic processes, E. Molinari and M. Tomellini 253 (2000) 367
- adsorption*
- Non-equilibrium vibrational kinetics in adlayers: outline of an alternative approach to catalytic processes, E. Molinari and M. Tomellini 253 (2000) 367
- desorption*
- Non-equilibrium vibrational kinetics in adlayers: outline of an alternative approach to catalytic processes, E. Molinari and M. Tomellini 253 (2000) 367
- surface excitations*
- Non-equilibrium vibrational kinetics in adlayers: outline of an alternative approach to catalytic processes, E. Molinari and M. Tomellini 253 (2000) 367
- catalysis*
- Non-equilibrium vibrational kinetics in adlayers: outline of an alternative approach to catalytic processes, E. Molinari and M. Tomellini 253 (2000) 367

*Thermodynamic and transport properties*

- Nuclear quadrupole coupling constant of  $^{21}\text{Ne}$  in the neon dimer and its influence on the  $T_1$  NMR relaxation time in fluid neon, A. Halkier, B. Kirchner, H. Huber and M. Jaszuński 253 (2000) 183

*Structure of solids, liquids and glasses*

- Topological properties of the hydrogen-bond network in liquid water, D.L. Bergman 253 (2000) 267
- Monte Carlo simulation study of solvent effect on  $\text{Na}^+$  to  $\text{Li}^+$  ion mutation, H.-S. Kim 253 (2000) 305
- Temperature-dependent optical Kerr effect spectroscopy of chloroform in restricted geometries, B.J. Loughnane, A. Scodinu and J.T. Fourkas 253 (2000) 323

*Biomolecular structure–function relationships*

- The keto–amino/enol tautomerism of cytosine in aqueous solution. A theoretical study using combined discrete/self-consistent reaction field models, C. Alemán 253 (2000) 13

